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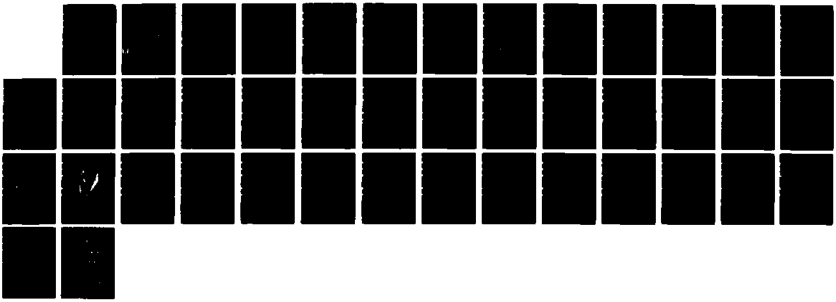

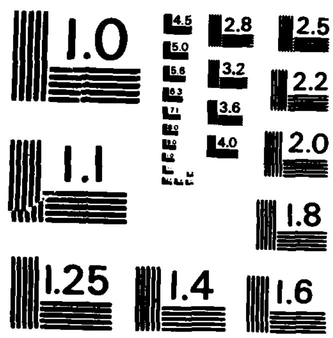

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NATIONAL BUREAU OF STANDARDS-1963-A

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TECHNICAL REPORT ARCCB-TR-85003

COMPUTER MODEL FOR THE SOLIDIFICATION OF COMPOSITION B

JOHN D. VASILAKIS

DECEMBER 1985

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT CENTER
CLOSE COMBAT ARMAMENTS CENTER
BENÉT WEAPONS LABORATORY
WATERVLIET, N.Y. 12189-4050

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Explosive Compound

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A computer model of an explosive compound, Composition B, solidfying in an M155 mm artillery shell is presented. Shells having been cast with the compound are frequently found with cracks seriously affecting their use. By developing a two-dimensional temperature-dependent model of the solidification process, it is hoped that some of the reasons for the crack initiation can be found. A general purpose finite element program, ADINAT, is used to evaluate

(CONT'D ON REVERSE)

20. ABSTRACT (CONT'D)

the model. The properties of both the Composition B and steel shell are treated as functions of temperature, and the boundary conditions are considered to be functions of both temperature and time. While the crack initiation cannot be predicted, following the solidification front will give information towards understanding the process. The work will establish the transient temperature distributions and solidification front motions for the various boundary conditions used. An extension of this work, to be performed later, will consider the stresses in the solidfying shell and the residual stress state after solidification is complete. Keywords: Charts; TNT; RDX; numerical analysis.

TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

Page

ACKNOWLEDGEMENTS

The author would like to express his gratitude to Dr. D. Wiegand, Energetic Materials Division, AMMCOM for his support in providing material property data, and for several discussions relating to the work and this report. G. Pflegl and G. P. O'Hara, Benet Weapons Laboratory, LCWSL, AMMCOM are also acknowledged for their help in developing the finite element model for the problem. Support for this work was partially provided by the Energetic Materials Division, LCWSL, Dover, NJ.

INTRODUCTION

Composition B has been used as an explosive in artillery shells for many years. It is a mixture of 60 percent RDX and 40 percent TNT with some wax added. Although the explosive compound has been in use for several years, there are still some difficulties associated with it. References 1 through 3 describe these problems and the results of efforts undertaken to better understand Composition B behavior. Some of the problems cited involve sensitivity of the explosive in large caliber weapons under conditions of high accelerations and several incidences in the field attributed to cracking and/or base separations in the case munitions. The studies review and investigate the crystallography, phase diagrams, chemistry, thermal processes, etc. They also include an extensive reference list.

In this report, a model of the solidification of Composition B in an M155 artillery shell is developed and exercised using various boundary conditions simulating the actual casting process in a manufacturing environment and in a laboratory environment. The transient temperatures throughout the solidification and subsequent cooling period are computed, the solidification front is followed, and the growth of the solidifying explosive shell at any point within the artillery shell itself is monitored, as well as the change in temperature at any point for any of the boundary conditions. The numerical analysis is performed using the thermal section of a general purpose finite

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[1] Rauch, F. C. and Wainright, R. B., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1969.
[2] Rauch, F. C. and Colman, W. P., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, March 1970.
[3] Colman, W. P. and Rauch, F. C., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1971.

element program for nonlinear analysis, ADINA. This thermal part, ADINAT, has the capability to handle phase change. All properties are input as functions of temperatures when available. The material properties used in the program are given in the Appendix. Similar earlier works by Nordio (ref 4) using analytical techniques and in Reference 1 using a computer program developed by Battelle were used to help determine some of the heat transfer coefficients used here. Nordio used the solution for a slab to relate to the cylinder solution. The resulting solidification rate could be found using a set of charts.

The boundary conditions treated in this report are laboratory type conditions, a controlled slow-cool procedure, and an assumed plant type boundary condition. These are better described in a later section. In all cases there is a riser assumed. A riser is used in casting procedures to provide additional molten material to make up the shrinkage which would occur during solidification. The attempt then is made to control the freezing process so that the molten material in the riser can flow to any cavities which may try to form.

The computer program used cannot account for any shrinkages and therefore no voids can exist in the model. The phase change is assumed to occur at a constant temperature. The finite element program used does consider phase changes over temperature intervals and this may be used in future work.

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[1]Rauch, F. C. and Wainright, R. B., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1969.

[4]Nordio, A., "The Cooling and Solidification of Molten Composition B and the Causes of Shrinkage Cavitations in Cast-Loaded Shell," Samuel Feltmann Ammunition Laboratories, Picatinny Arsenal, Dover, NJ, AD69987, August 1955.

PROBLEM STATEMENT

The governing partial differential equation for a solidification process is given by

$$\frac{1}{r}\frac{\partial}{\partial r}\left[k(T) r \frac{\partial T}{\partial r}\right] + k(T)\frac{\partial T}{\partial z} = c(T)\rho(T)\frac{\partial T}{\partial t} \tag{1}$$

where T is temperature

k(T) is thermal conductivity, (BTU/in.°F hr)

c(T) is specific heat, (BTU/#°F)

$\rho(T)$ is density, (#/in.^{3})

At the phase change interface, the following boundary conditions must be satisfied (ref 5):

$$T = T_f \tag{2}$$

$$\Delta q^2 dS = \pm\ \rho L \frac{\partial v}{\partial t} \tag{3}$$

where T_f is phase change temperature

L is latent heat per unit mass of material being converted

v is volume of material being converted

Δq^2 is heat flow from the phase change interface

dS is element of interface area

The minus sign is for heat liberated as in solidification and the plus sign for heat absorbed as in melting.

Equation (3) states that the amount of heat being liberated due to the solidification is proportional to the volumetric rate of conversion, and this

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[5]Rolph III, W. D. and Bathe, K.-J., "An Efficient Algorithm For Analysis of Nonlinear Heat Transfer With Phase Change," Int. Journal Num. Methods in Engineering, Vol. 18, No. 1, January 1982.

is balanced by the heat flow Δq^2 out of the interface between the liquid and solid region. The boundary conditions are of the form

$$\frac{\partial T}{\partial r} - h(T-T_{amb}) = 0 \tag{4}$$

where h is a convective heat transfer coefficient. The method used in ADINAT to construct the latent heat flow vector is the enthalpy method. This method alters the enthalpy of the system to account for the latent heat.

These equations (1) through (4) are solved using the finite element program ADINAT. The finite element grid that was used in the analysis is shown in Figure 1. The problem was assumed to be axisymmetric so that only one-half of the structure need be shown. Four node quadrilateral elements were used, each one representing a ring of material. The outer three elements on the bottom and right side represent the artillery shell. There are 536 nodal points and 477 elements, 315 of which represent the explosive fill.

BOUNDARY CONDITIONS

The solidification of Composition B in a 155 mm artillery shell was studied for three different sets of boundary conditions. The first boundary conditions modeled were taken from Reference 3. These represent an experimental attempt to control the solidification under laboratory conditions while at the same time monitoring the transient temperatures in the explosive as it cools. The boundary conditions are reproduced here from the report for the 155 mm model.

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[3]Colman, W. P. and Rauch, F. C., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1971.

The cooling bath is initially at 160°F and covers the lower half of the shell. The upper portion is heated with 190°F water circulating through a coil. After pouring the explosive, a flow of 120°F water is introduced into the bath to a height of 12 inches, and in time, the following occurs.

Time After Pouring (Hours)	Event
4-1/2	Bath water level raised from 12" to 16"
6	Bath water level raised to 20", the 190°F water in upper heating coil shut off.
7-1/2	120°F water to bath shut off. Bath remains stagnant while cooling to ambient temperature.

The total time to cool was about 20-24 hours. The desired effect of this procedure was to have the Composition B solidify upward from the base of the artillery shell. In the figures, these are indicated as "Laboratory Conditions".

A second set of boundary conditions initially considers the shell (initially at 160°F) to be placed in a 184°F bath after pouring. The explosive is also assumed to be at 184°F. The bath temperature is then slowly decreased to 168°F in four hours, with the intention of slowly solidifying the explosive in the shell. The bath temperature is then slowly cooled to an ambient temperature of 65°F in 24 hours total time. This set of boundary conditions would try to simulate a very slow, controlled solidification process and is called "Slow Cool" in the figures.

The third set of boundary conditions discussed in this report tries to model what could occur during a production process. The artillery shell is assumed to be initially at 65°F. The melt is assumed to be 184°F. The explosive is poured into the shell, the shell is covered with a shroud and then allowed to slowly cool to room temperature. These are called "Plant Conditions".

RESULTS

Figures 2 through 9 show the results from the first set of boundary conditions. These try to model the laboratory experiment described in the previous section and are labeled "Laboratory Conditions". The figures show the cooling versus time for selected points in the material. Some contour plots and three-dimensional plots at specific times are also presented. Figure 2 shows the temperature-time cooling curves for three selected locations at the axis of the shell. These are the nodes nearest the points 6.5 inches, 11.625 inches, and 16.75 inches from the artillery shell base, and are noted L, M, and U in the figure respectively and are also shown in Figure 1. The dimensions are the locations of thermocouples used in the laboratory castings of Reference 3. Although the onset of solidification is delayed about one hour in the model output depicted here compared with the laboratory results (ref 3), the results of the model seem to compare well with other aspects of the experiment. The delay mentioned is probably due to quantifying the boundary conditions from Reference 3, although accurate knowledge of thermophysical properties and constants is always difficult and can add to the discrepancy. The three points do cool in the expected manner, however, in that the point nearest the base (L), solidified first, followed by the central

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[3]Colman, W. P. and Rauch, F. C., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1971.

section (M), and finally the top (U). One can see that the temperature of the material remains constant until the latent heat is given up and that point begins to cool again. Occasionally, cooling is too rapid for this to be noticed. No shrinkage can be allowed in the model, hence, a riser is assumed to maintain a full shell. The explosive solidifies in approximately the same time interval and the cooling to room temperature continues as it appears in the laboratory test. Figure 3 shows the solidification results of other nodes located along the lower part of the axis and of the shell. Node 1 has a height 0.68 inch above the base of the shell, at the interface of the explosive and the shell, and node 73 is 3.9 inches from the base. Locations of these nodes are also shown in Figure 1. Figure 4 shows similar solidification curves for points on the axis, but at the upper end of the shell. The curve indicated by node 217 is at a height of 11.83 inches from the shell base and by node 361 at the top of the shell (where the riser starts). The solidification does not appear to occur as progressively upward along the axis as one would like. This is because the boundary conditions are not continuously changed in time in that the water level is subject to step changes and the upper part of the shell has less material to cool and solidify. Therefore, when the water level is raised, the cross-section of the shell with the smallest diameter wants to cool first. Figure 5 shows what is happening on a cross-section of the shell at a height of 11.83 inches. The cooling of several nodes is shown from the axis of the shell to a point in the Composition B at the shell wall. One can see that the temperature of this point follows the imposed boundary conditions. One can also see the time it takes to solidify through to the axis.

Figure 6 is two separate attempts to show information on the temperature distribution in the Composition B at a specific time during the solidification process, which in this case is 3.2 hours. The bath water height is at 12 inches and at 120°F. The figure on the left represents contour lines or lines of constant temperature within the Composition B. The outermost outline would represent the outline of the Composition B inside the shell. Only the right half is shown here as the problem is treated as axisymmetric (the other side would be a mirror image of the half shown) and the figure is bounded on the left by the shell axis. Temperature values of the contours are noted in the accompanying chart. The 'S' contour represents the solidification front. The right side of Figure 6 shows the temperature distribution in the Composition B plotted as a surface. Nose and base labels on the contour plot and on the three-dimensional plot try to indicate the orientation and view of the three-dimensional plot. The explosive in both the upper and lower parts of the shell has solidified. The center plot portion of the shell (3-D plot) shown as a plateau, appears to be bounded by a shape similar to the solidus contour. With regard to the labeling in the lower part of the figure, NCON, NX, and NY relate to the grid and PHI and THETA are orientation angles for the three-dimensional plot. For the other variables TAB represents ambient temperature, TMELT is the temperature at which the explosive solidifies, both in degrees Fahrenheit, and TIME is the time past since the initial filling of the shell. Figure 7 shows the same type of view early in the process (time = 0.1 hour). One can see from the plateau in the three-dimensional plot and from the contour plot that solidification is just beginning near the lower part of the shell wall and at the base of the shell. The contour line is not identifiable here. The material within the contour levels crowded near the boundary, especially at the box, however, should be in a solid state.

In Figure 8 the time in the cooling cycle is 6.2 hours. It should be stated that it was not possible to model the exact boundary conditions from Reference 3. There are several unknowns including the amount of heat being taken away from the base of the projectile, the exact length of the upper heating coil, the rate at which the 160°F bath water cooled when the 120°F water was introduced, etc. The figure, however, does point out some interesting effects. Initially, the bath water is 12 inches from the base and 4.5 hours into the cooling cycle, it is raised to a height of 16 inches. These levels can both be identified in the three-dimensional plot by observing the valley indicated by A in the figure. One can also see that the solidification process has not been completed in the lower part of the shell and some liquid still remains near the axis near the area labeled B. On the three-dimensional plot, this is the level near the work axis. The unlabeled contour line (solidus lines) can also be seen surrounding Y in the upper portion of the shell, indicating that the material between it and the axis is still molten.

Finally, Figure 9 shows the results at a time of 11.2 hours. The shell has solidified and appears to be uniformly cooling to room temperature.

Cooling curves for the second set of boundary conditions, indicated by "Slow Cool," are given by Figures 10 through 13. These figures show cooling curves at the same points in the explosive as in the previous case. Figure 10

[3] Colman, W. P. and Rauch, F. C., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1971.

represents the cooling curves at three locations along the axis in the shell. The response of a point near the base is indicated by L, in the central section by M, and in the upper section by U. Since the projectile is placed in a constant temperature bath and the bath temperature is decreased uniformly along the height of the projectile, the upper section of the shell solidified first, having less material in that section. Figure 11 shows the cooling curves for a set of points located on the lower part of the shell axis. The cooling curve nearest 1 is at the base of the shell and the distance from the base increases as curve 73 is approached. The curve 'L' in Figure 9 would correspond to a location in the shell near curve 73 so that the curves shown represent cooling nearer the base. Solidification occurs early for the curve nearest 1 which is at the shell base. One can see the temperature hold at the solidus temperature until the latent heat is dissipated for any of the points. Figure 12 shows the results for points along the axis in the upper section of the shell and Figure 13 for points across a cross-section at a height of 11.8 inches. Again, Figure 13 shows the temperature changes along a cross-section at a certain height. Each curve represents the cooling in time of a point located in the cross-section.

The final set of results using boundary conditions labeled "Plant Conditions" is shown in Figures 14 through 17. Here, the shell is assumed to be at 65°F, the explosive melt poured in, and a shroud put over the shell to slow the solidification. Free convection heat transfer was assumed in estimating the convection heat transfer coefficients used in the model. Figure 14 again compares results in the lower, middle, and upper sections of the shell axis. Since the shell surface temperatures are not controlled by cooling baths as in the two previous cases, the cooling curves take a more natural shape. Again, however, the node in the upper section solidifies first. Figure 15 shows solidification curves for nodes on the lower part of the axis and Figure 16 for nodes in the upper part of the axis. Finally, Figure 17 shows the response of the set of nodes at a cross-section 11.8 inches from the base.

CONCLUSIONS

Because of the shape of the shell, it is difficult to force the Composition B to solidify from the base of the shell to the top as can be seen from the results of the first set of boundary conditions. The slow-cool boundary conditions, although similar contour and three-dimensional plots are not included here, would show a more uniform solidification front. However, the Composition B solidifies from the top down and a void would probably occur at some distance near the base depending on how quickly the base itself is cooled. The plant conditions probably present an idealistic view of what actually happens. Here, also, the solidification is from the top towards the base.

The laboratory type boundary conditions might provide more uniform results if the water level could be slowly and continuously raised and the coil maintaining the explosive in the liquid state could be long enough to surround the entire length of the projectile. Thus initially, the coil would extend to the entire length of the shell and there would be no water in the bath. As the water enters, the coil is withdrawn to allow solidification. This would be done gradually and at a rate that allows solidification throughout the plane at that water level.

The slow-cool boundary conditions would probably work quite well if the shell could be inverted. The riser would now be at the base of the shell with the solidification front in the right direction so voids along the centerline could be avoided. One might also introduce an additional barrier to heat flow in the smaller diameter sections of the shell such as a high temperature plastic or composite jacket, fitting tightly over the shell to prevent the bath coolant from contacting the shell. The shell can then be cooled in a slow-cool type environment. The jacket could be of varying thickness to guarantee freezing from the base toward the top of the shell.

REFERENCES

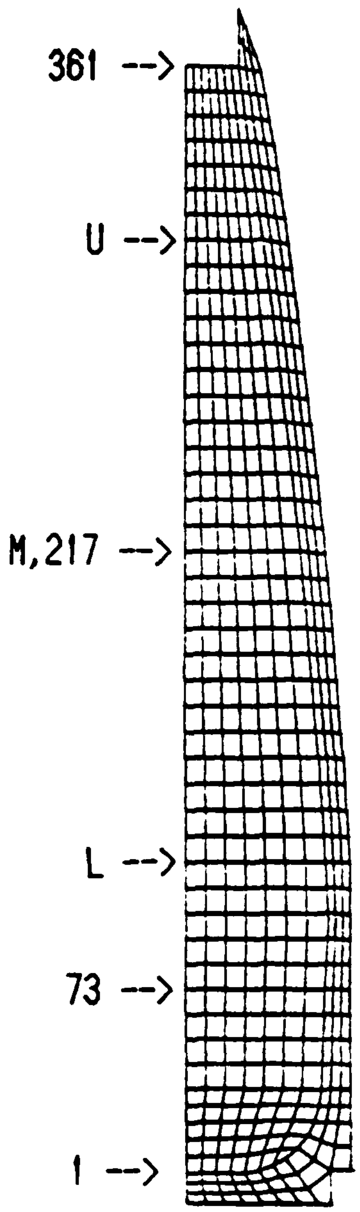
1. Rauch, F. C. and Wainright, R. B., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1969.

2. Rauch, F. C. and Colman, W. P., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, March 1970.

3. Colman, W. P. and Rauch, F. C., "Studies on Composition B," Final Report, Picatinny Arsenal, Dover, NJ, February 1971.

4. Nordio, A., "The Cooling and Solidification of Molten Composition B and the Causes of Shrinkage Cavitations in Cast-Loaded Shell," Samuel Feltmann Ammunition Laboratories, Picatinny Arsenal, Dover, NJ, AD69987, August 1955.

5. Rolph III, W. D. and Bathe, K.-J., "An Efficient Algorithm For Analysis of Nonlinear Heat Transfer With Phase Change," <u>Int. Journal Num. Methods in Engineering</u>, Vol. 18, No. 1, January 1982.



NUMBERS AND LETTERS SHOW NODES AND LOCATIONS ALONG THE AXIS WHICH ARE REFERRED TO IN THE TEXT AND FIGURES

FIGURE 1. FINITE ELEMENT GRID MODEL OF M155 SHELL AND EXPLOSIVE

SOLIDIFICATION OF COMPOSITION B
(LABORATORY CONDITIONS)

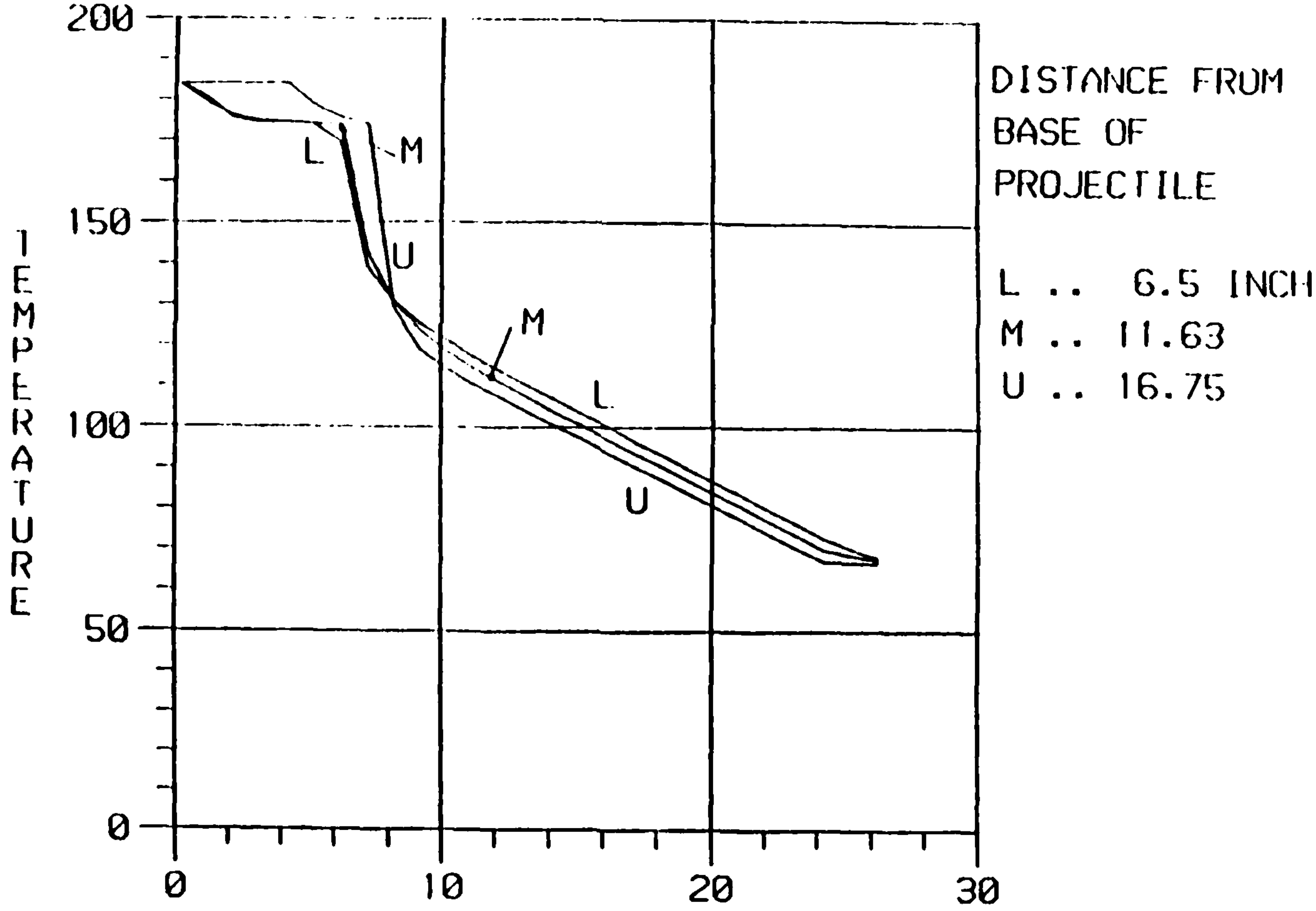


FIGURE 2

SOLIDIFICATION OF COMPOSITION B

(LABORATORY CONDITIONS)

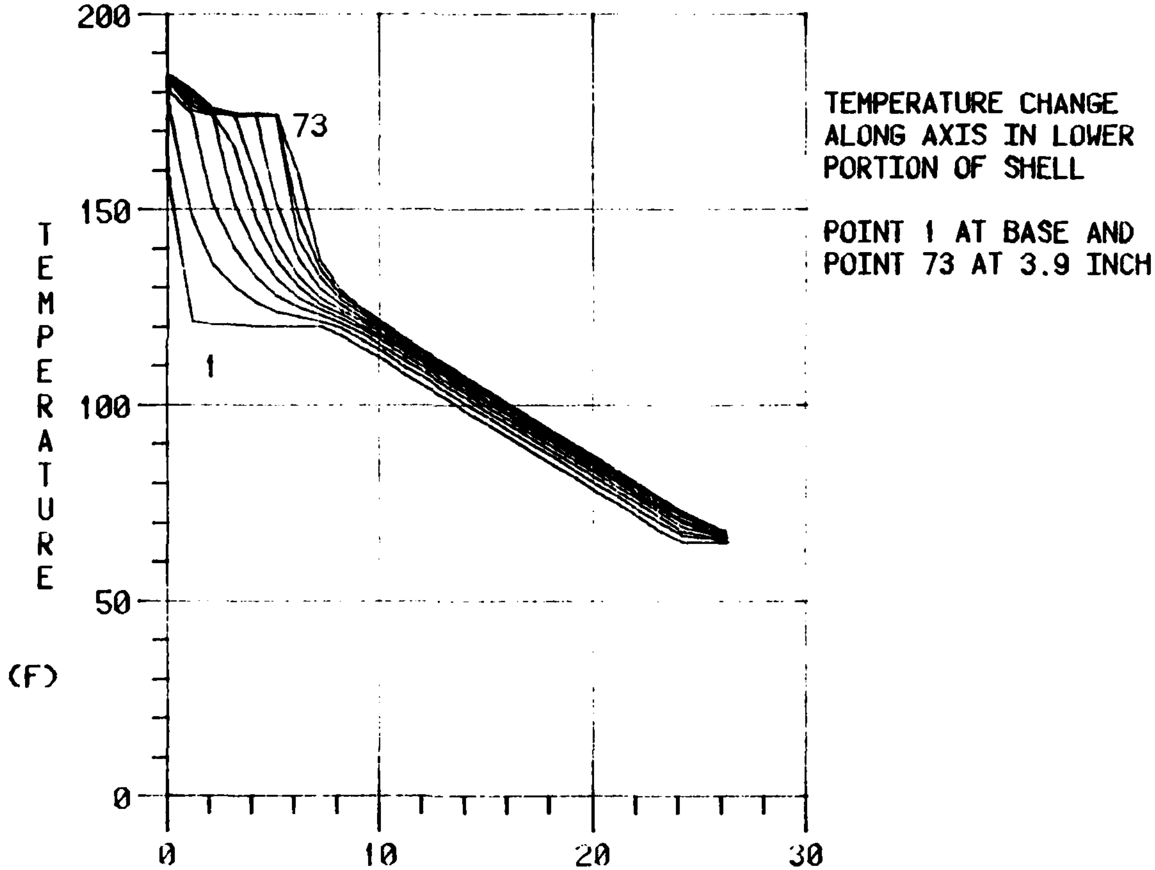


FIGURE 3

SOLIDIFICATION OF COMPOSITION B

(LABORATORY CONDITIONS)

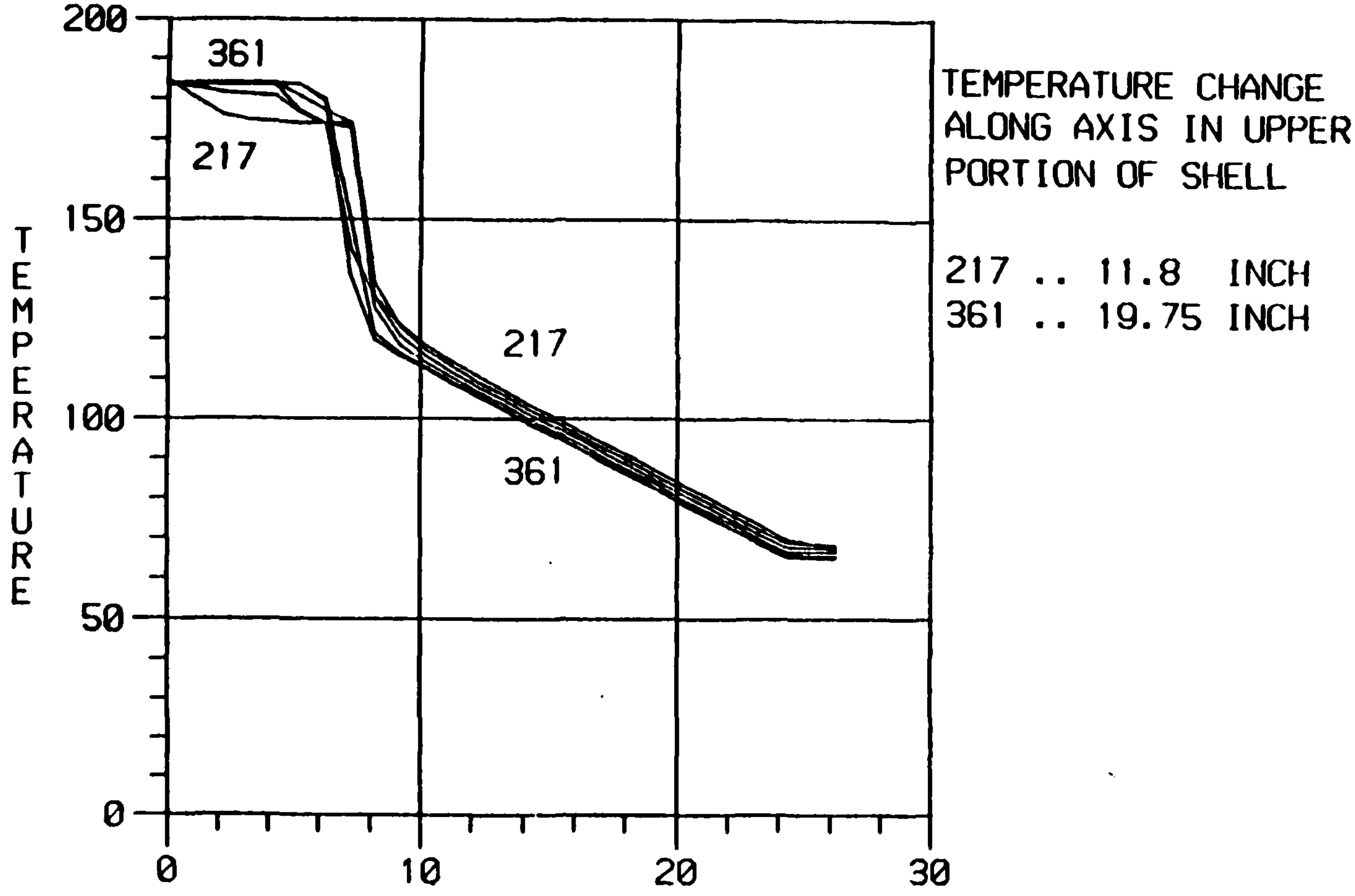


FIGURE 4

SOLIDIFICATION OF COMPOSITION B

(LABORATORY CONDITIONS)

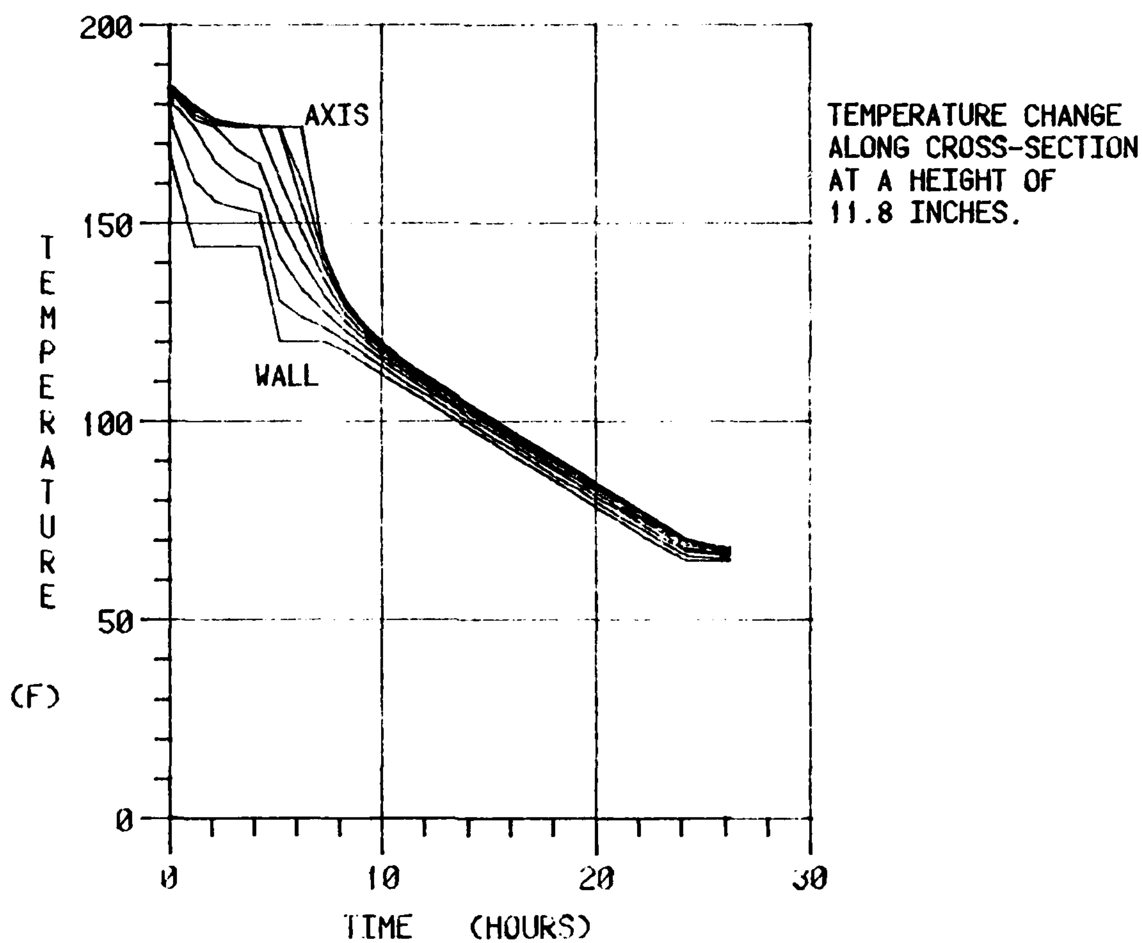
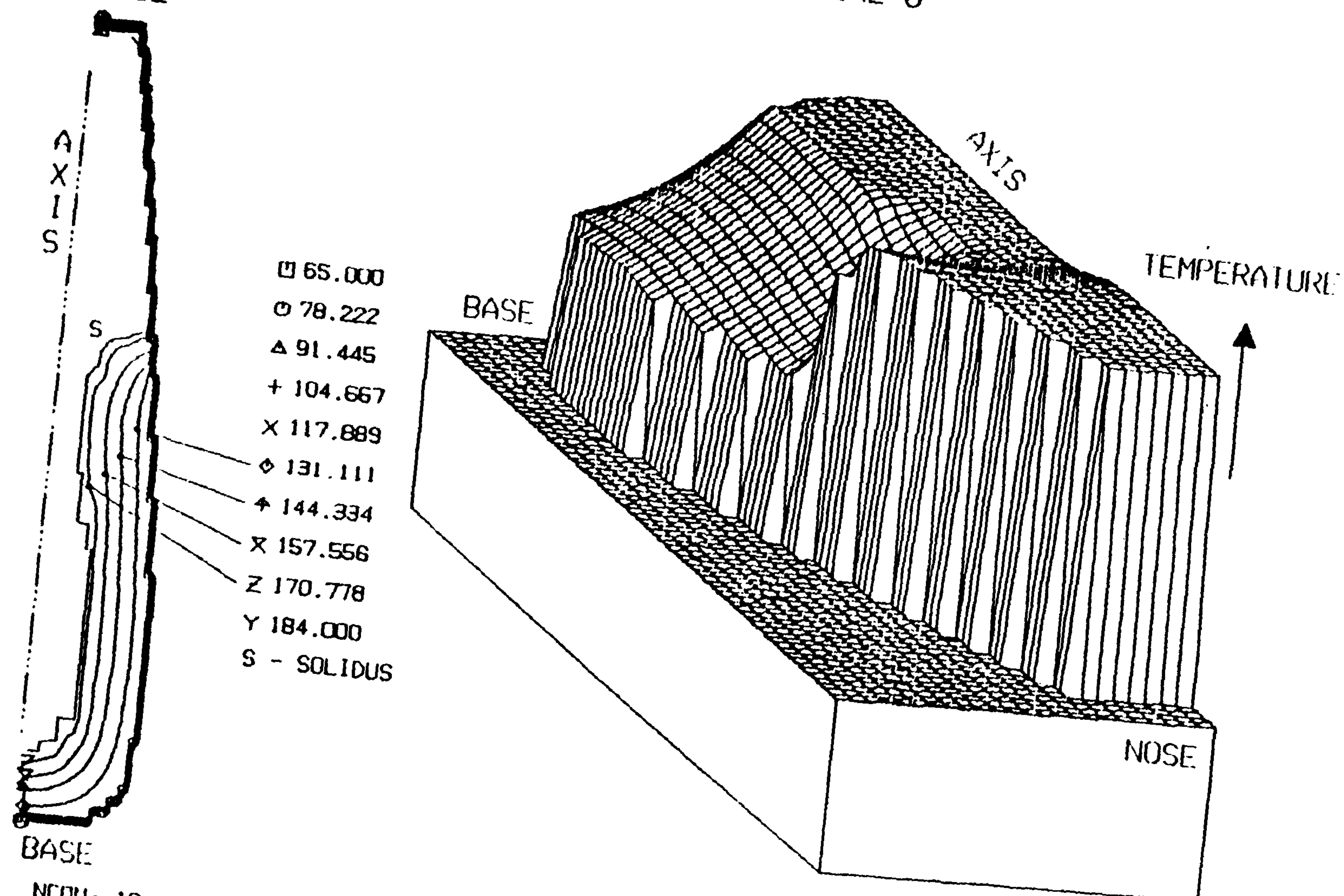


FIGURE 5

LABORATORY CONDITIONS

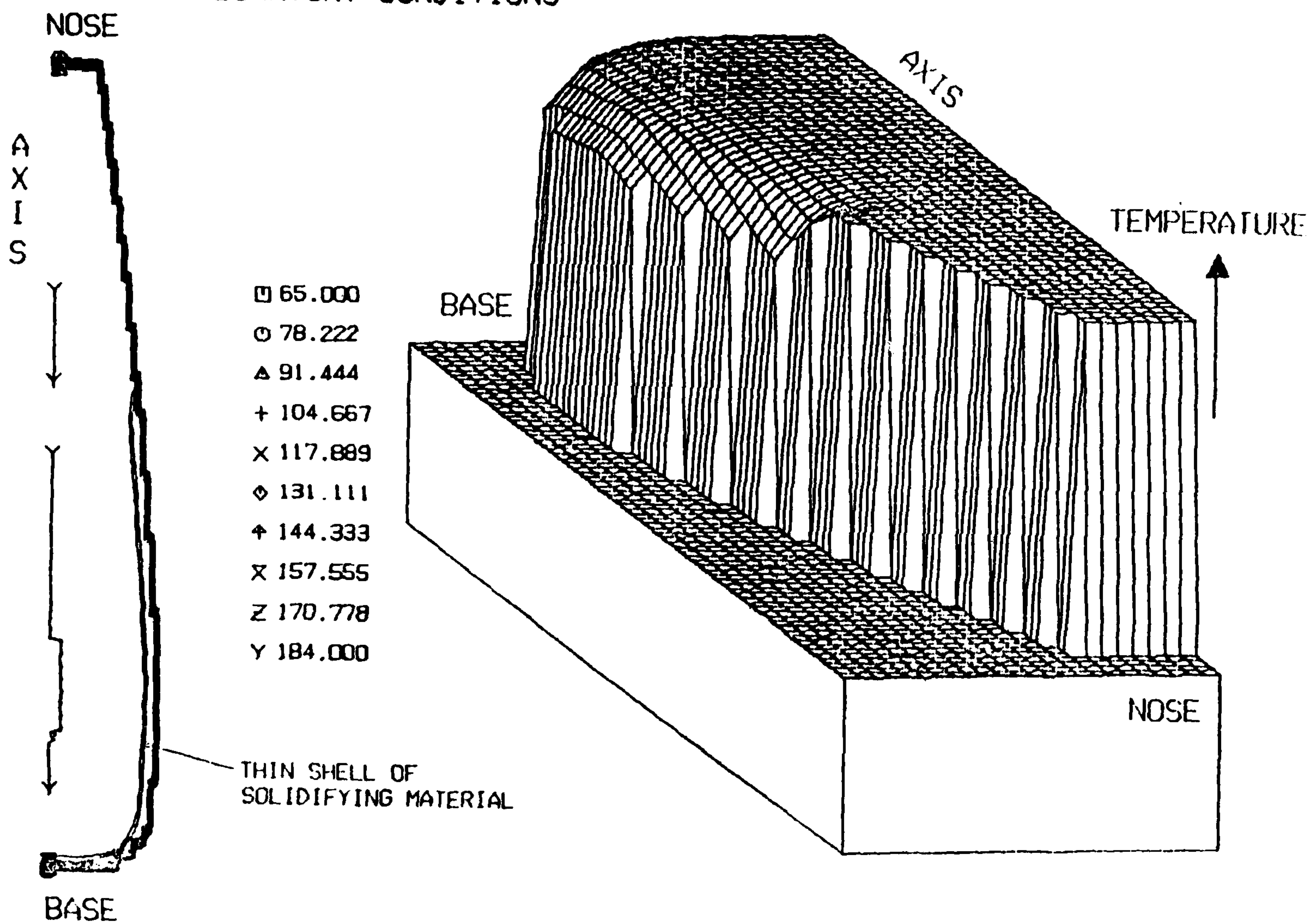
FIGURE 6



NCON=-10, NX=25, NY=73, TAMB=65.0, TMELT=174.2, PHI=190.0, THETA=350.0, TIME(HR)=3.2
TEMPERATURE DISTRIBUTION IN COMPOSITION B

FIGURE 7

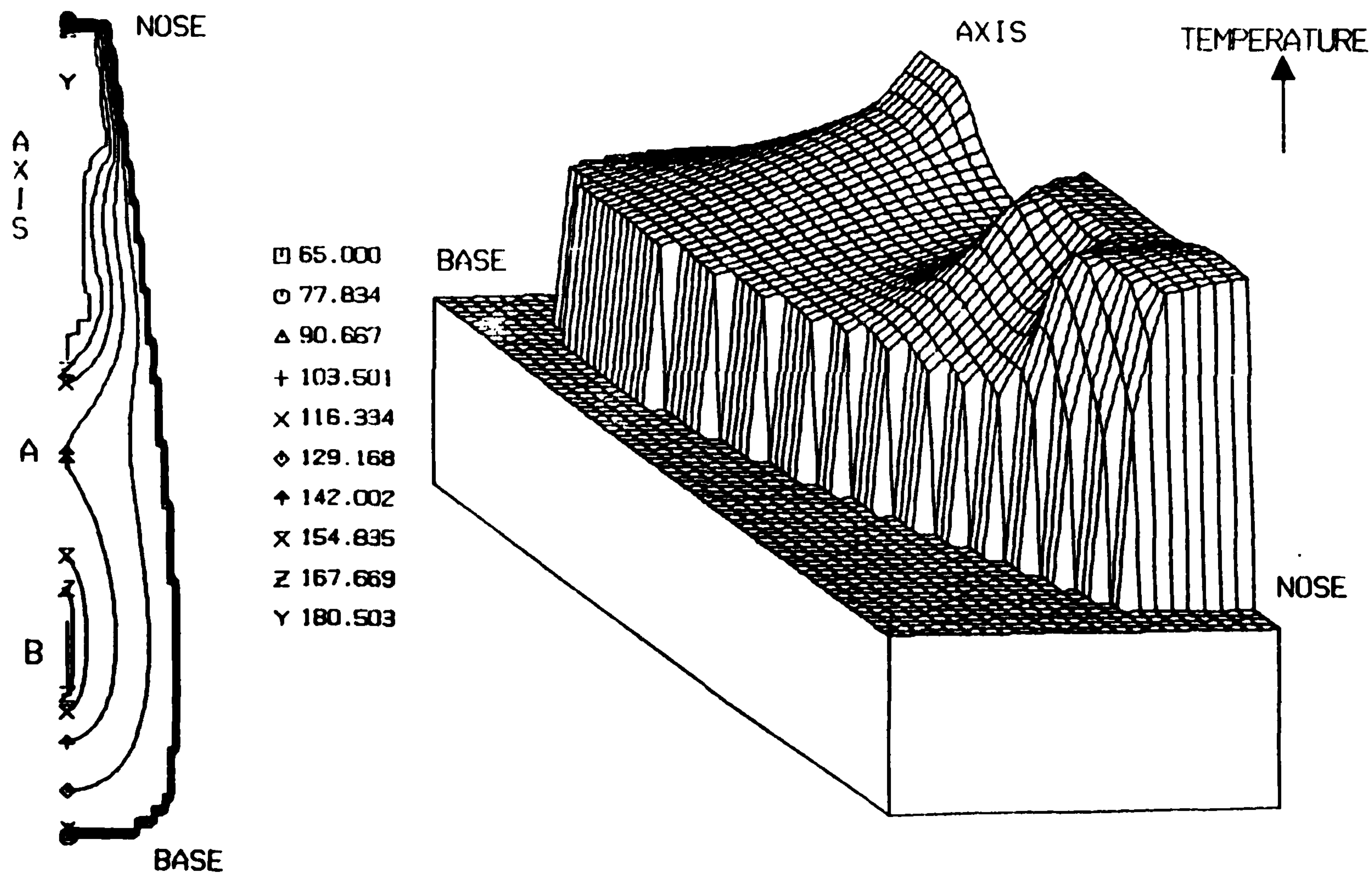
LABORATORY CONDITIONS



NCON=-10. NX=25. NY=73. TAMB=65.0. TMELT=174.2. PHI=190.0. THETA=350.0. TIME(HR)=0.1
TEMPERATURE DISTRIBUTION IN COMPOSITION B

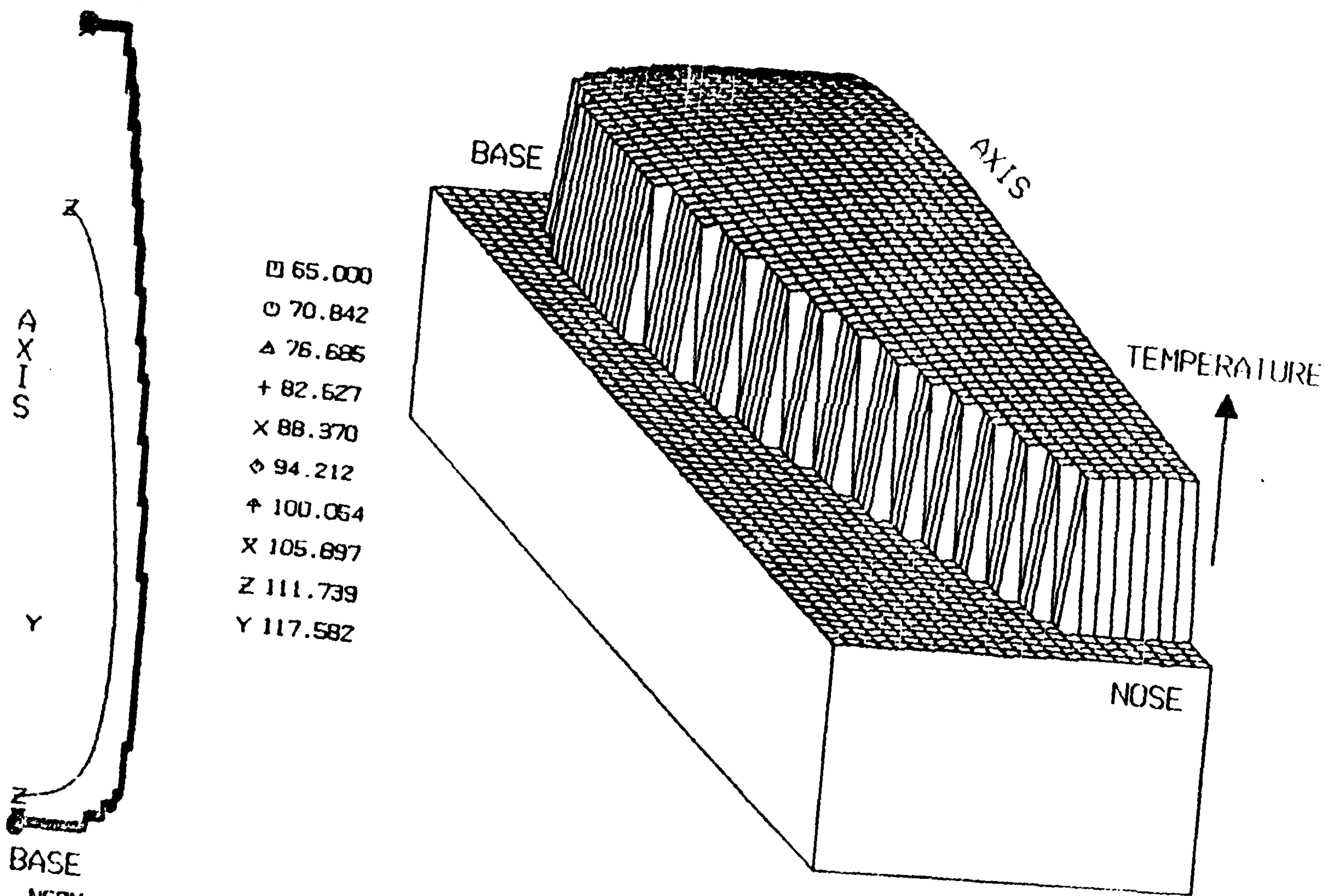
LABORATORY CONDITIONS

FIGURE 8



NCON=-10. NX=25. NY=73. TAMB=65.0. TMELT=174.2. PHI=190.0. THETA=350.0. TIME(HR)=6.2
TEMPERATURE DISTRIBUTION IN COMPOSITION B

LABCRATORY CONDITIONS FIGURE 9



NCON=-10. NX=25. NY=73. TAMB=65.0. TMELT=174.2. PHI=190.0. THETA=350.0. TIME(HR)=11.2
TEMPERATURE DISTRIBUTION IN COMPOSITION B

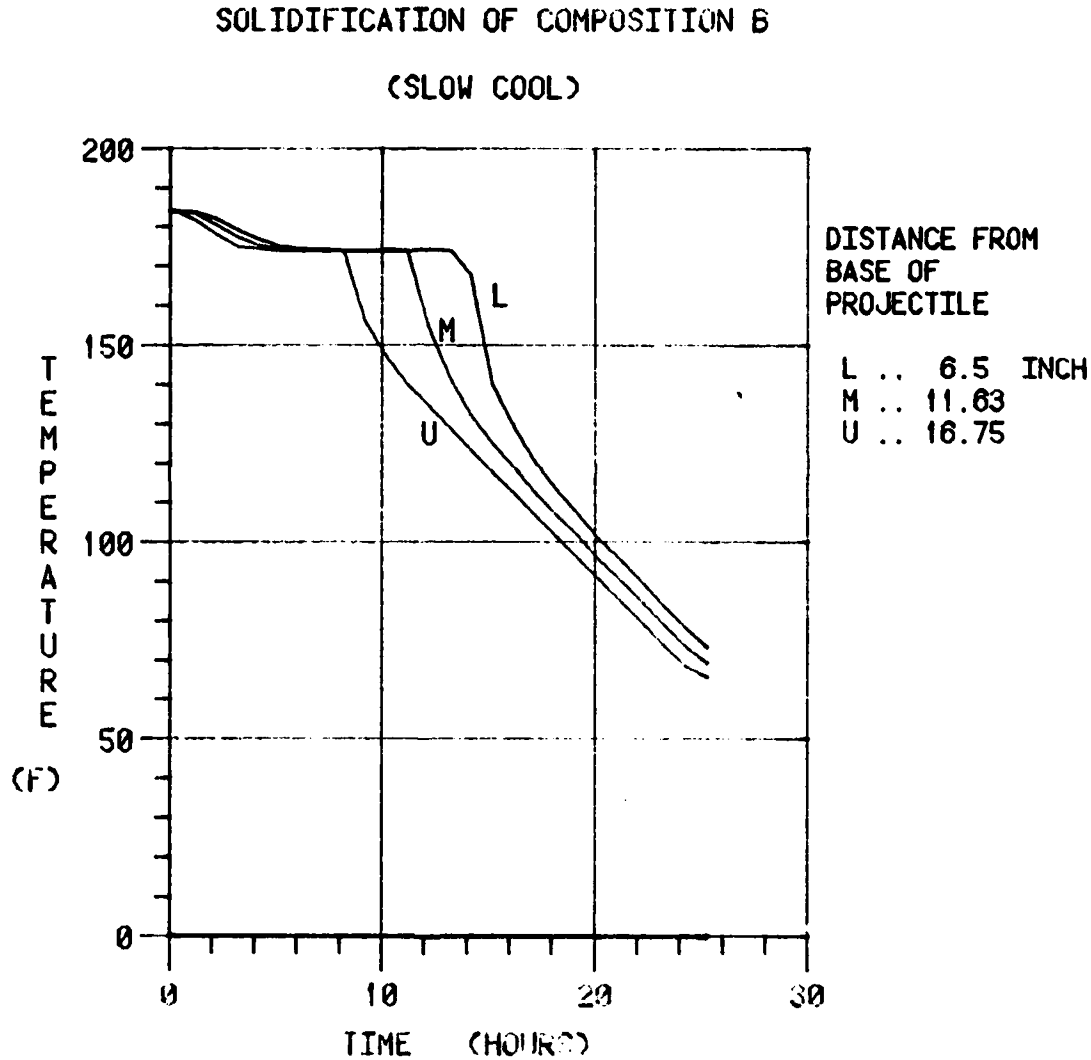

SOLIDIFICATION OF COMPOSITION B
(SLOW COOL)
TEMPERATURE (F)
200
150
100
50
0
TIME (HOURS)
0
10
20
30
L
M
U
DISTANCE FROM BASE OF PROJECTILE
L .. 6.5 INCH
M .. 11.63
U .. 16.75

FIGURE 10

SOLIDIFICATION OF COMPOSITION B

(SLOW COOL)

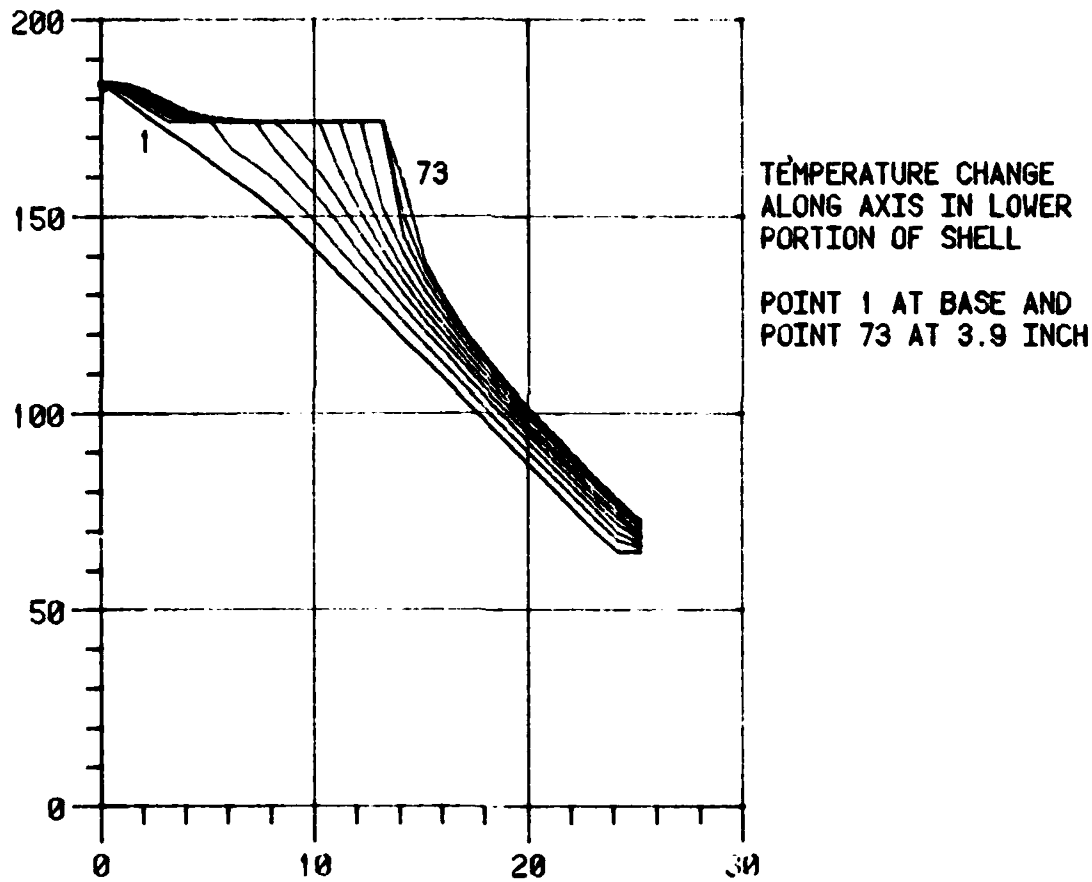


FIGURE 11

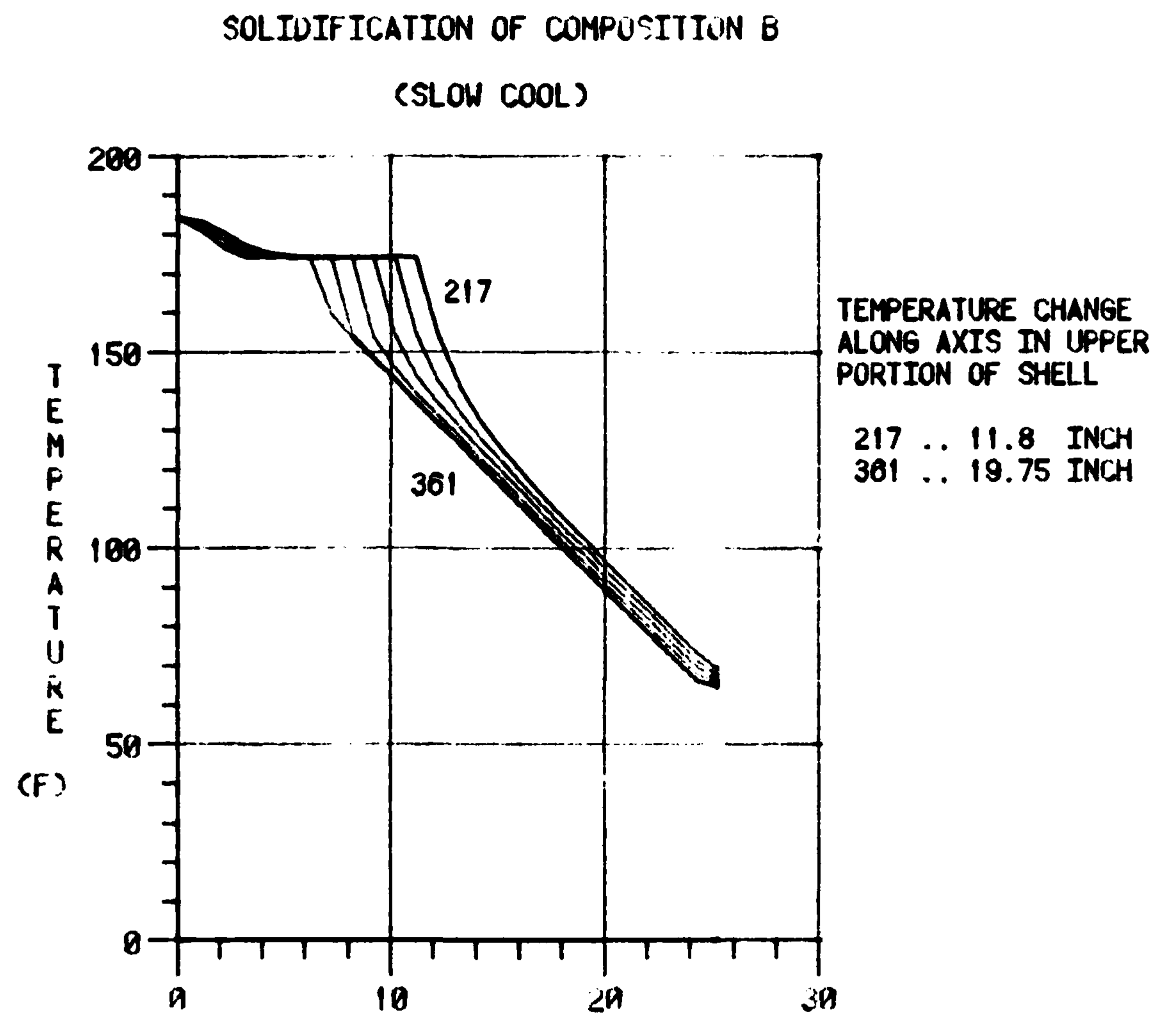

SOLIDIFICATION OF COMPOSITION B
(SLOW COOL)
200
150
100
50
0
TEMPERATURE
(F)
0
10
20
30
TIME (HOURS)
217
361
TEMPERATURE CHANGE
ALONG AXIS IN UPPER
PORTION OF SHELL
217 .. 11.8 INCH
361 .. 19.75 INCH

FIGURE 12

SOLIDIFICATION OF COMPOSITION B

(SLOW COOL)

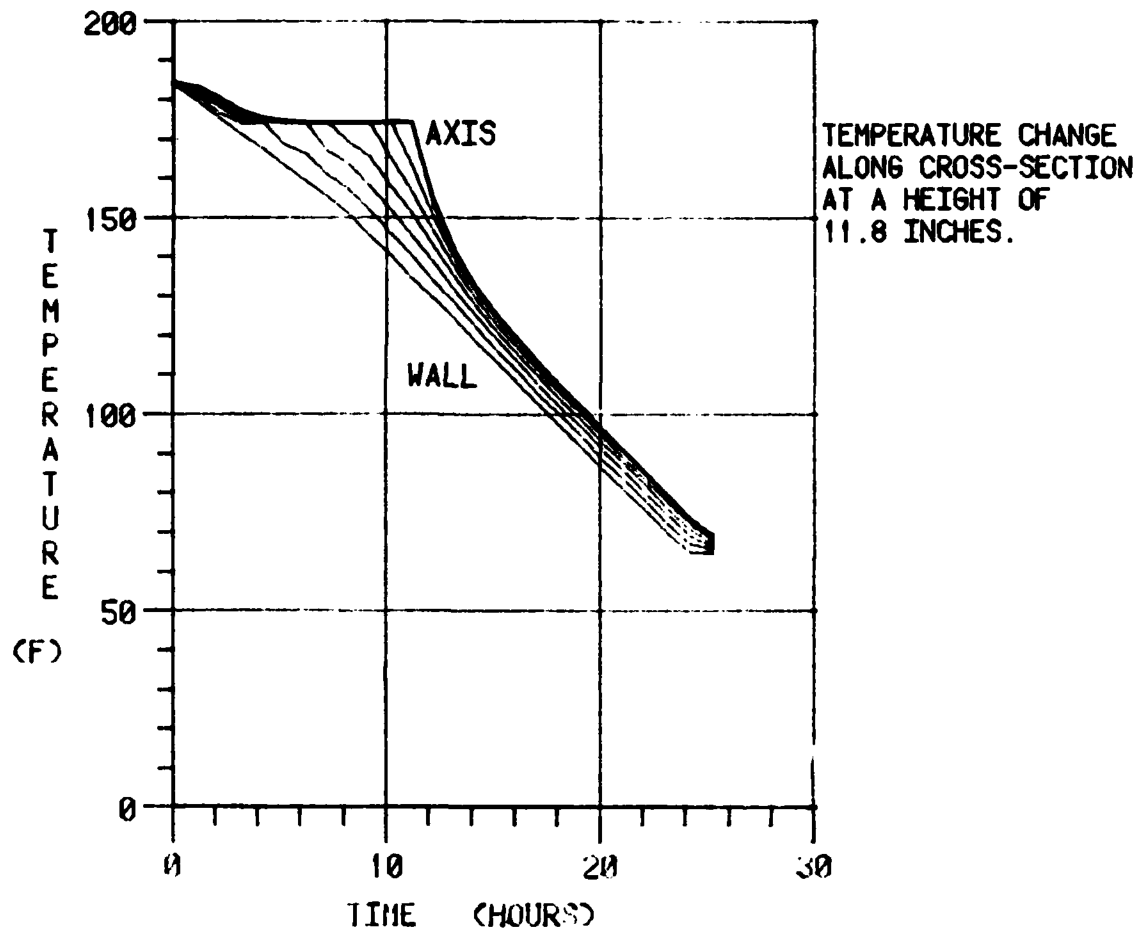


FIGURE 13

SOLIDIFICATION OF COMPOSITION B

(PLANT CONDITIONS)

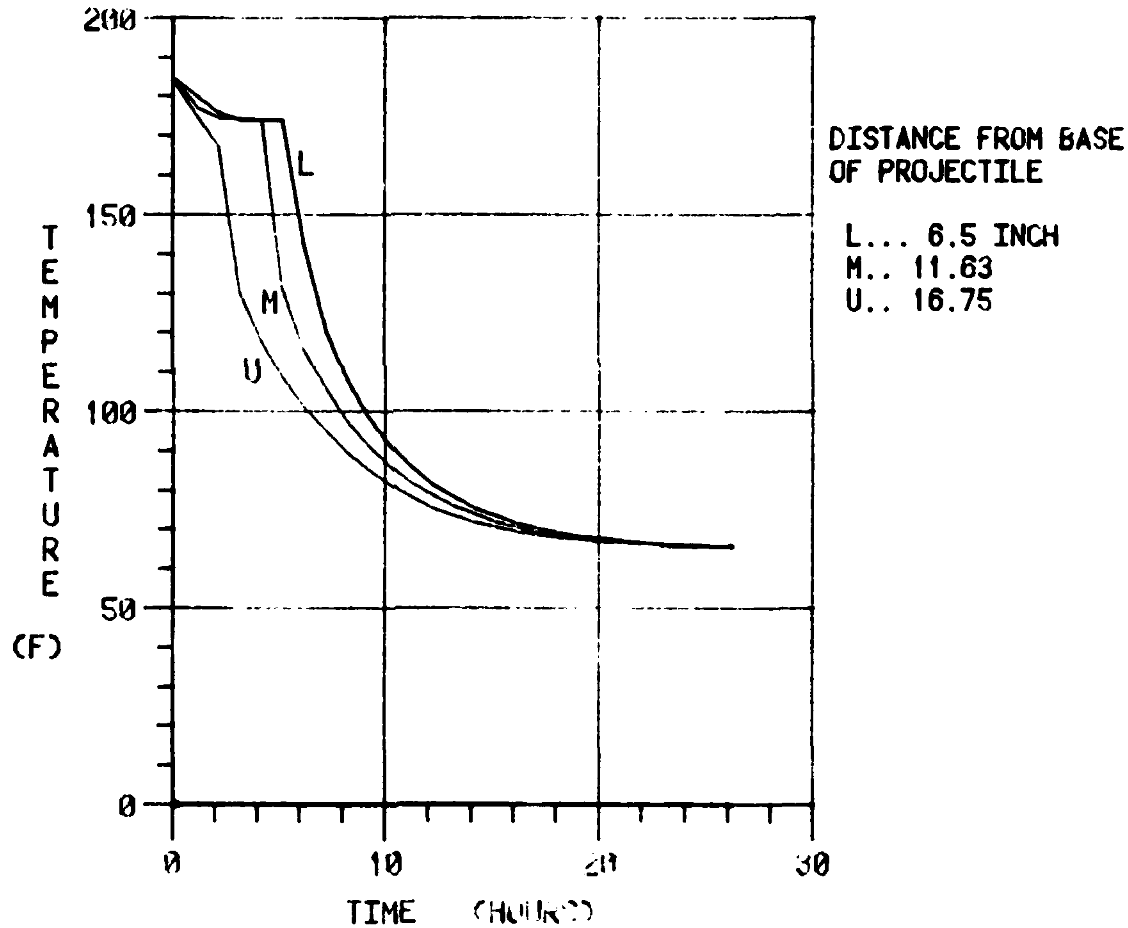


FIGURE 14

SOLIDIFICATION OF COMPOSITION B

(PLANT CONDITIONS)

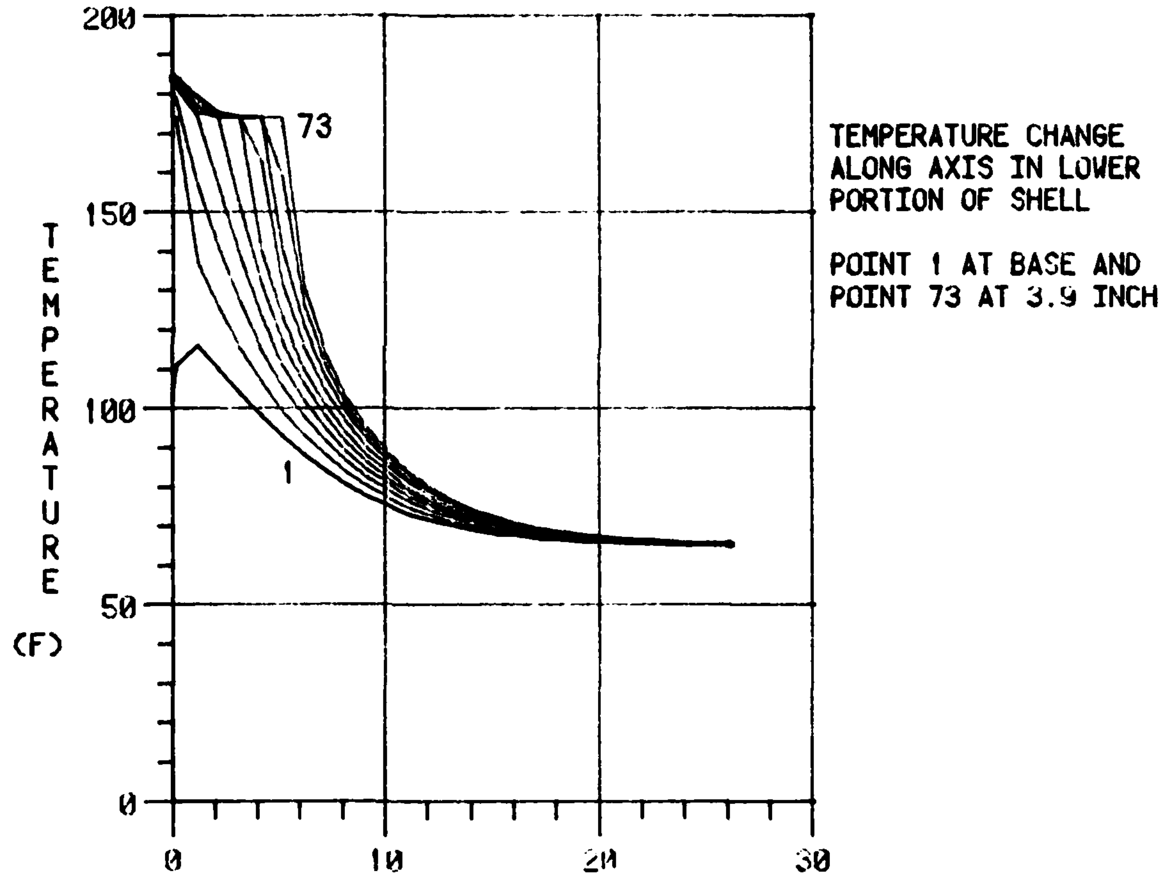


FIGURE 15

SOLIDIFICATION OF COMPOSITION B

(PLANT CONDITIONS)

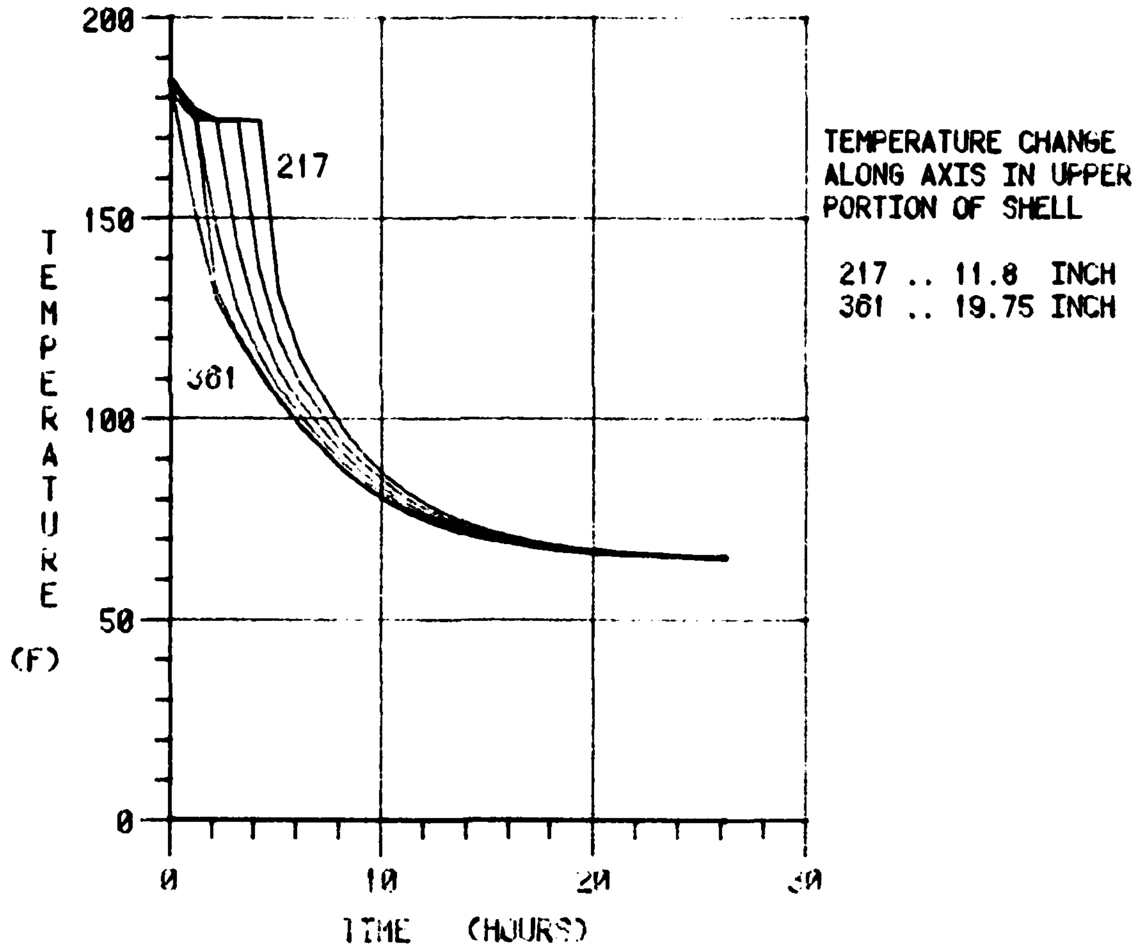


FIGURE 16

SOLIDIFICATION OF COMPOSITION B

(PLANT CONDITIONS)

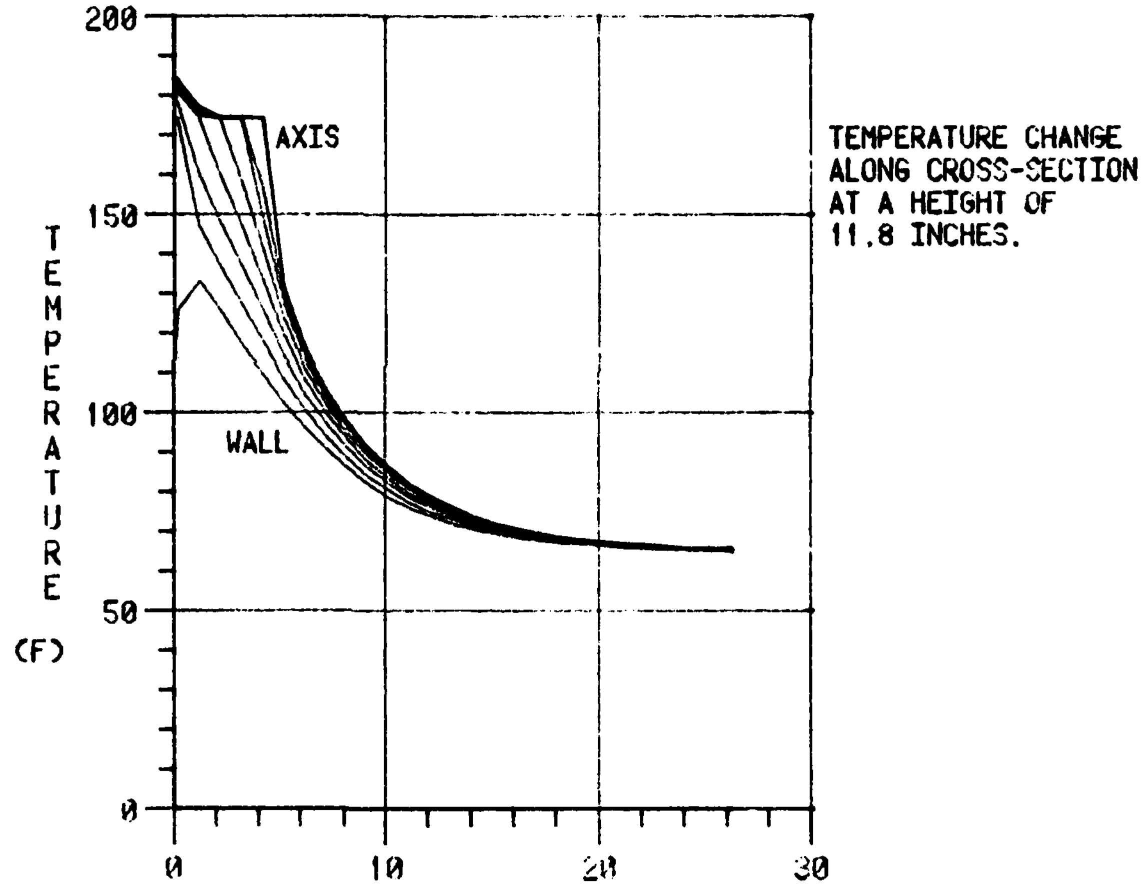


FIGURE 17

APPENDIX

MATERIAL PROPERTIES

The tables below show the material properties used in the program. The program linearly interpolates between temperatures.

	COMPOSITION B	
Temperature °F	Thermal Conductivity BTU/hr °F in.	Specific Heat BTU/in.^{3}
0.0	.01152	.0143
45.	-	.018
174.1	.01152	-
174.3	.01325	-
200.	.01325	-
207.	-	.0202

	STEEL CASE	
Temperature °F	Thermal Conductivity BTU/hr °F in.	Specific Heat BTU/in.^{3}
0	1.8036	.0298
200	1.8	-
400	1.7748	-
1300	-	.0523

The latent heat of the Composition B was taken to be 1.51 BTU/#.

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